Dirac equation in (1+2) dimensions for quasi-particles in graphene and quantum field theory of their Coulomb interaction.

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Abstract

There is evidence for existance of massless Dirac quasi-particles in graphene, which satisfy Dirac equation in (1+2) dimensions near the so called Dirac points which lie at the corners at the graphene's brilluoin zone. Certain subtle points which are peculiar to odd number of space-time dimensions (in this case three), in the derivation of such an equation are clarified. It is shown that parity operator in (1+2) dimensions play an intersting role and can be used for defining conserved chiral currents [there is no γ^5 in (1+2) dimensions] resulting from the underlying Lagrangian for massless Dirac quasi-particles in graphene which is shown to have chiral $U_L(2) \times U_R(2)$ symmetry. Further the quantum field theory (QFT) of Coulomb interaction of 2D graphene is developed and applied to vacuum polarization and electron self energy and the renormalization of the effective coupling of this interaction and Fermi velocity.

Recently there has been a lot of interest in graphene. On experimental side it has some anomalous magnetic and transport properties[1]. On theoretical side its low energy excitations are massless, chiral Dirac fermions[1]. This implies existence of quasi-particles in graphene, which satisfy massless Dirac equation in (1+2) dimensions near the so called Dirac points which

lie at the corners of graphene's Brilluoin zone. This is indicated by energy dispersion around the Dirac point given by [1]

$$E_{\pm} \simeq \pm v_f \,|\mathbf{q}| + O(|\mathbf{q}|^2) \tag{1}$$

which reminds one of relativistic energy-momentum relation for massless or ultra relativistic particles although Fermi velocity is three hundred times smaller than the speed of light. The derivation of such an equation given in literature [1,2] is in the form

$$i\boldsymbol{\sigma}.\boldsymbol{\nabla}\psi = E\psi \tag{2}$$

where $\boldsymbol{\sigma} = (\sigma^1,\, \sigma^2)$ and $\boldsymbol{\nabla} = (\frac{\partial}{\partial x^1}, \frac{\partial}{\partial x^2}\ )$, which has two dimensional form of the usual Dirac equation for two component left-handed or right-hand massless fermions and not exactly in the form of Dirac equation in (1+2) dimensions[see below]. The purpose of this paper is to clarify such points and to disscuss the subtleties of odd [in this case three] space-time dimensions and develop a quantum field theory of Coulomb interaction of 2D graphene.

In graphene for the hexagonal layer the unit cell contains two atoms A and B, belonging to two sublattices. The lattice vectors are [1]

$$\mathbf{a}_1 = \frac{a}{2}(3, \sqrt{3}), \qquad \mathbf{a}_2 = \frac{a}{2}(3, -\sqrt{3}) \tag{3}$$

where $a \simeq 1.42A^0$ is the carbon-carbon distance.

The Dirac points K and K$'$ have their postion vectors in momentum space:

$$\mathbf{K} = \frac{2\pi}{3a}(1, \sqrt{3}), \qquad \mathbf{K}' = \frac{2\pi}{3a}(1, -\sqrt{3}) \tag{4}$$

In the tight binding approach, the Hamiltonion is given by [1]

$$\mathcal{H} = -t \sum_{<i,j>} (a_i^\dagger b_j + h.c.) \tag{5}$$

where $a_i(a_i^\dagger)$ are annihilation(creation) operators for an electron in sub-lattice A with an equivalent definition for sub-lattice B. $t(\simeq$ 2.8eV)is the nearest hopping energy (hopping between different sub-lattices)

Let us expand the Hamiltonian (5) at any of two independent lattice points[2], which we may take as given in Eq. (3), around the Dirac point K$'$. This gives

$$\delta\mathcal{H} = \begin{pmatrix} 0 & \delta\mathcal{H}_{AB} \\ \delta\mathcal{H}^*_{AB} & 0 \end{pmatrix}$$

where

$$\mathcal{H}_{AB} = -t[e^{i\mathbf{k}.\mathbf{a}_1} + ie^{i\mathbf{k}.\mathbf{a}_2}] \tag{6}$$

Writing

$$\mathbf{k} = \mathbf{K}^{'} + \mathbf{q}$$

and expanding around $K^{'}$ keeping terms linear in $|\mathbf{q}|$,

$$\delta\mathcal{H}_{AB} = \frac{3at}{2}[iq_x + q_y] \tag{7}$$

This gives

$$\begin{aligned} \delta\mathcal{H} &= \begin{pmatrix} 0 & iq_x + q_y \\ -iq_x + q_y & 0 \end{pmatrix} \\ &= v_f[-q^1\sigma^2 + q^2\sigma^1] \end{aligned} \tag{8}$$

where $v_f = \frac{3at}{2}$ is the Fermi velocity, σ^1 and σ^2 are Pauli matrices, $q^i = (q^1, q^2)$, in relativistic notation: $q^\mu = (q^0, q^1, q^2)$. This does not give $\boldsymbol{\sigma}.\mathbf{q}$ as implied in Eq. (2). The Eq. (8) can be put in the form

$$\begin{aligned} \delta\mathcal{H} &= v_f[i\sigma^3\sigma^1 q^1 + i\sigma^3\sigma^2 q^2] \\ &= \gamma^0(\boldsymbol{\gamma}.\mathbf{q}v_f) \end{aligned} \tag{9}$$

where $\gamma^0 = \sigma^3$, $\gamma^1 = i\sigma^1$, $\gamma^2 = i\sigma^2$ are Dirac matrices in (1+2) dimensions. The above is the Dirac Hamiltonian for massless fermion in (1+2) dimensions near the Dirac point $K^{'}$. The corresponding Dirac equation is

$$\mathcal{H}\psi = E\psi_{\pm}, \qquad E = \pm v_f\,|\mathbf{q}| \tag{10}$$

or

$$i\frac{\partial\psi}{\partial t} = \gamma^0(\boldsymbol{\gamma}(-i\boldsymbol{\nabla}v_f)\psi \tag{11}$$

Writing $\partial_0 = \frac{1}{v_f}\frac{\partial}{\partial t}$, we can write the Eq (10) in covariant form

$$i(\gamma^0\partial_0 + \gamma^1\partial_1 + \gamma^2\partial_2)\psi = 0$$

or

$$i(\gamma^\mu\partial_\mu)\psi = 0 \tag{12}$$

which is the Driac equation in (1+2) dimensions for a massless fermion[3].

It is important to remark that if we expand around the Dirac point K, we obtain

$$\begin{aligned} \delta\mathcal{H} &= v_f[-q^1\sigma^2 - q^2\sigma^1] \\ &= v_f[i\sigma^3\sigma^1 q^1\sigma^1 - i\sigma^3\sigma^2 q^2] \end{aligned} \tag{13}$$

Now it is known [3] that in 3 space-time dimensions there exists two inequivalent representations for γ-matrices [this is true for any odd number of space-time dimensions]:

$$\begin{aligned} \gamma^0 &= \sigma^3,\ \gamma^1 = i\sigma^1, \gamma^2 = i\sigma^2 \\ \gamma^0 &= \sigma^3,\ \gamma^1 = i\sigma^1, \gamma^2 = -i\sigma^2 \end{aligned} \tag{14}$$

We have used the first of these represantations for the expansion around the Dirac point K$'$. We take the second representation for the expansion around the Dirac point K, whcih is obtained from K$'$ by the parity operation, defined by the matrix[3]

$$\Lambda = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{pmatrix} \tag{15}$$

so that $\det\Lambda = -1$. Thus we see that under the parity operation

$$q^1 \longleftrightarrow q^1,\ q^2 \longleftrightarrow -q^2 \text{ and } \delta\mathcal{H}_K \longleftrightarrow \delta\mathcal{H}_{K'}$$

Taking the two representations mentioned above into account we can write the parity conserving Lagrangian[3] as

$$\mathcal{L} = \overline{\psi}_+(i\partial)\psi_+ + \overline{\psi}_-(i\widetilde{\partial})\psi_-$$

where

$$\begin{aligned} \partial &= \gamma^0\partial_0 + \gamma^1\partial_1 + \gamma^2\partial_2 \\ \widetilde{\partial} &= \gamma^0\partial_0 + \gamma^1\partial_1 - \gamma^2\partial_2 \end{aligned} \tag{16}$$

Parity operation takes the solutions in one representation to the other:

$$\begin{aligned} \psi_+^p(x^p) &= -\eta_p\psi_-(x) \\ \psi_-^p(x^p) &= -\eta_p\psi_+(x) \end{aligned} \tag{17}$$

where $x^p = (x^0, x^1, -x^2)$. It is convenient to transform to new fields[3]

$$\begin{aligned} \psi_A &= \psi_+ \\ \psi_B &= i\gamma^2\psi_- \end{aligned} \quad (18)$$

The Lagrangian (16) can then be written as [3]

$$\mathcal{L} = \overline{\psi}_A(i\gamma^\mu\partial_\mu)\psi_A + \overline{\psi}_B(i\gamma^\mu\partial_\mu)\psi_B \quad (19)$$

where under partiy operation now

$$\begin{aligned} \psi_A^p(x^p) &= -i\eta_p\gamma^2\psi_B(x) \\ &= \eta_p\sigma^2\psi_B(x) \\ \psi_B^p(x^p) &= -i\eta_p\gamma^2\psi_A(x) \\ &= \eta_p\sigma^2\psi_A(x) \end{aligned} \quad (20)$$

In (1+2) dimensions, there is no γ^5 available as in (1+3) dimensions. But still we may define

$$\psi_{L,R} = \frac{\psi_A \pm \psi_B}{\sqrt{2}} \quad (21)$$

so that the Lagrangian (19) takes the form

$$\mathcal{L} = \overline{\psi}_L i\gamma^\mu\partial_\mu\psi_L + \overline{\psi}_R i\gamma^\mu\partial_\mu\psi_R \quad (22)$$

This Lagrangian is invariant under two independant chiral transformations

$$\psi_L \to e^{i\alpha_L}\psi_L, \ \psi_R \to e^{i\alpha_R}\psi_R \quad (23)$$

where α_L and α_R are real, and has thus $U_L(2) \otimes U_R(2)$ symmetry. The corresponding conserved currents are

$$\begin{aligned} J_L^\mu &= \overline{\psi}_L\gamma^\mu\psi_L \\ J_R^\mu &= \overline{\psi}_R\gamma^\mu\psi_R \end{aligned} \quad (24)$$

We can develop quantum field theory for Coulomb interaction of 2D graphene in analogy with QED (for another approach see [2,4]). The "free" Hamiltonian as implied by Eq. (11) is

$$\mathcal{H}_o = v_f \int d^2r\psi^\dagger(\mathbf{r})\gamma^o\boldsymbol{\gamma}.(-i\boldsymbol{\nabla})\psi(\mathbf{r}) \quad (25)$$

$$v_f \int d^2r\overline{\psi}(\mathbf{r})\boldsymbol{\gamma}.(-i\boldsymbol{\nabla})\psi(\mathbf{r}) \quad (26)$$

The instantaneous Coulomb interaction in 2D graphene is

$$\mathcal{H}_I = \frac{e^2}{2} \int d^2x_1 d^2x_2 \frac{n(t,\mathbf{x}_1)n(t,\mathbf{x}_2)}{4\pi\left|\mathbf{x}_1 - \mathbf{x}_2\right|} \tag{27}$$

where $n(t,\mathbf{x}_1) = \psi^\dagger(t,\mathbf{x}_1)\psi(t,\mathbf{x}_1) = \overline{\psi}(t,\mathbf{x}_1)\gamma^o\psi(t,\mathbf{x}_1)$. This gives the scattering matrix element between four fermions

$$S_{fi}^{coulomb} = -ie^2\frac{1}{2}\int dt \int d^2x_1 \int d^2x_2 \frac{< f|n(t,\mathbf{x}_1)n(t,\mathbf{x}_2)|i >}{4\pi\left|\mathbf{x}_1 - \mathbf{x}_2\right|} \tag{28}$$

The integral can be written as $\int d^Dx_1 d^Dx_2 \delta(t_2 - t_1)$ where $D = 3$ in (1+2) dimensions. Expanding ψ's into creation and annihilation operators, one finally abtains [5]

$$iT_{fi} = \frac{1}{4\pi v_f}[\overline{u}(p_2')(-ie\gamma^\mu)u(p_2)\frac{i\eta_\mu\eta_\nu}{2[-q^2+(q.\eta)^2]^{\frac{1}{2}}}\overline{u}(p_1')(-ie\gamma^\mu)u(p_1) - \text{crossed term}] \tag{29}$$

where $\frac{1}{2|\mathbf{q}|}$, $|\mathbf{q}| = [-q^2+(q.\eta)^2]^{1/2}$is Fourier transform of $\frac{1}{4\pi|\mathbf{x}_1-\mathbf{x}_2|}$ in two space dimensions, $\eta^\mu = (1,0,0)$, so that $\eta_\mu\gamma^\mu = \gamma^o$ and longitudnal photon momentum may be taken as $l^\mu \equiv 2(q^\mu - \eta.q\eta^\mu)$, $\mu = 0,1,2$; so that $(-l^2)^{1/2} = 2\left|\mathbf{q}\right|$.

Thus we may write Feynman rules for 2D coulomb interaction in analogy with QED as follows:

(i) Vertex factor: $-ie\gamma^\mu$,

(ii) Internal lines

Photon ("longitudinal") line: $\frac{i\eta_\mu\eta_\nu}{2[-q^2+(q.\eta)^2]^{\frac{1}{2}}}$

(iii) Spin$\frac{1}{2}$ massless fermion: $\frac{i}{\not{p}}$

$\not{p} = \gamma^\mu p_\mu$ $\mu = 0,1,2$, this follows from the Lagrangian given in Eq. (19).

As an application of these rules, we calculate vacuum polarization $\text{II}(q^2) = \eta_\mu\eta_\nu\ \text{II}^{\mu\nu}(q)$, which arizes from photon self energy due to fermion loop. It is given by

$$-i\text{II}^{\mu\nu}(q) = (-1)\frac{1}{v_f}\int \frac{d^Dl}{(2\pi)^D} Tr[(-ie\gamma^\mu)\frac{i}{\not{l}+i\epsilon}(-ie\gamma^\nu)\frac{i}{\not{l}+2(\not{q}-q.\eta)\ \not{\eta}+i\epsilon}], \tag{30}$$

The integration will be done by using Feynman parametrization and dimensional regularization. The singular terms combine to give $(1-\frac{D}{2})\Gamma(1-\frac{D}{2}) =$

$\Gamma(2-\frac{D}{2})$, i.e. finite answer, which however cancels with a similar term in the trace. The net result is

$$\mathrm{II}^{\mu\nu}(q^2) = \frac{e^2}{v_f}\frac{1}{(2\pi)^{\frac{D}{2}}}(D+\frac{1}{2})\Gamma(2-\frac{D}{2})\int_0^1 dx\sqrt{x(1-x)}\frac{A_{\mu\nu}}{2\Delta} \tag{31}$$

where $(D+\frac{1}{2})$ arizes from the trace for odd space time dimensions, $\Delta = [(q.\eta)^2 - q^2]^{\frac{1}{2}} = |\mathbf{q}|$ and

$$A_{\mu\nu} = -8g^{\mu\nu}((q.\eta)^2 - q^2) - 8q^\mu q^\nu + 8q.\eta(q^\mu\eta^\nu + \eta^\nu q^\mu - (q.\eta)\eta^\mu\eta^\nu) \tag{32}$$

Using $D=3$, we finally get

$$\begin{aligned}
\mathrm{II}(q^2) &= \eta_\mu\eta_\nu \mathrm{II}^{\mu\nu} = \frac{e^2}{8v_f}(\Delta) \\
&= \frac{e^2}{4\pi v_f}\left|\mathbf{q}\right|\frac{\pi}{2} \\
&= g\frac{\pi}{2}\left|\mathbf{q}\right|,
\end{aligned} \tag{33}$$

in agreement with the known result [6], where $g = \frac{e^2}{4\pi v_f}$ is the dimensionless [in units $\hbar = 1$] effective coupling constant.

We now discuss how the vacuum polarization renormalizes the interaction coupling constant. For this purpose we consider the response of charged fermion to an externally applied field [Coulomb potential in two space dimensions in momentum space is$A_o = -\frac{e}{2|\mathbf{q}|} = \eta_\mu A^\nu$, where $A^\nu = (-\frac{e}{2|\mathbf{q}|}, \mathbf{0})$], namely

$$\overline{u}(ie\gamma^\mu)u\frac{i\eta_\mu\eta_\nu}{2\Delta}A_\nu \tag{34}$$

which is modified to

$$\begin{aligned}
&\overline{u}(ie\gamma^\mu)u\frac{i\eta_\mu\eta_\nu}{2[\Delta + \mathrm{II}(q^2)]}A_\nu \\
&= -\frac{e^2}{2\left|\mathbf{q}\right|}\overline{u}\gamma^0 u\frac{1}{1+\frac{g\pi}{2}} \\
&= -g\frac{4\pi v_f}{2\left|\mathbf{q}\right|}\frac{1}{1+\frac{g\pi}{2}}
\end{aligned} \tag{35}$$

where we have used Eq. (33). Thus the renormalized g, often written as g_{sc} [6] is

$$g_{sc} = \frac{g}{1+\frac{g\pi}{2}} \tag{36}$$

The implications of this result are discussed in [6]. It is instructive to calculate fermion self energy which is given by

$$-i\Sigma(p)=\frac{1}{v_f}\int\frac{d^3l}{(2\pi)^3}(-ie\gamma^\mu)\frac{i}{\not l}(-ie\gamma^\nu)\frac{i\eta_\mu\eta_\nu}{2\left|\mathbf{l}-\mathbf{p}\right|} \tag{37}$$

After making the Wick rotation $l^0=il_E^0$ (E for Euclidean matric) and carrying out the l_E^0 integration (which occurs only in fermion propagator), which gives $\pi\frac{1}{|\mathbf{l}|}$, the rest of integration is in $D=2$ dimension. Using Feynman parametrization

$$\frac{1}{a^{1/2}b^{1/2}}=\frac{1}{\pi}\int_0^1 x^{-1/2}(1-x)^{-1/2}\frac{1}{ax+b(1-x)}, \tag{38}$$

and the dimensional regularization one obtains

$$-i\Sigma(p)=-\frac{ie^2}{16\pi v_f}(-\not\eta\boldsymbol{\gamma}\cdot\mathbf{p}\not\eta)\ln\frac{\Lambda^2}{\left|\mathbf{p}\right|^2} \tag{39}$$

where we have used

$$\frac{1}{(4\pi)^{(D/2-1)}}\frac{\Gamma(1-D/2)}{\Gamma(1)}\left(\frac{1}{L}\right)^{1-D/2}=\left[\frac{2}{\varepsilon}-(\ln L+\gamma-\ln 4\pi)\right]$$

with $L=\left|\mathbf{p}\right|^2x(1-x)$, $\frac{2}{\varepsilon}$ signifies the ultraviolet log divergence: $\ln\Lambda^2$.

Noting that

$$\begin{aligned}-\not\eta\boldsymbol{\gamma}\cdot p\not\eta &= \boldsymbol{\gamma}\cdot\mathbf{p}=-\not p+\gamma^0p^0\\ \Sigma(p) &= \frac{g}{4}\left[-\not p+\gamma^0p^0\right]\ln\frac{\Lambda}{|\mathbf{p}|}\end{aligned} \tag{40}$$

where $p^0=v_f\left|\vec{p}\right|$ is the energy. The usual interpretation of this result is that coefficient of second term in parenthesis gives the radiative correction to energy

$$E=v_f\left|\mathbf{p}\right|Z_2^{-1} \tag{41}$$

where

$$Z_2^{-1}=1+\frac{g}{4}\ln\frac{\Lambda}{|\mathbf{p}|} \tag{42}$$

The coefficient of $\not p$ gives the renormalization of the electric charge, $e\rightarrow Z_2e$,which however is cancelled by the corresponding contribution from the

vertex part by the use of Ward Identity. The vacuum polarization correction is finite and renormalize g to g_{sc} as given in Eq. (36). The result (41) is interpreted as renormalization of the fermi velocity v_f [2,4,6]. This equation is important for the renormalization group analysis of g and v_f [4,6].

In summary we have clarified the derivation of Dirac equation for quasi-particles in graphene in (1+2) dimensions near the Dirac points K$'$ and K. The role of two inequvalent representations of Dirac matrices in (1+2) dimensions [a property of odd number of space-time dimensions] visa vis parity operation is emphasised. It is shown that the underlying Lagrangian for quasi-particles in graphene has chiral $U_L(2) \otimes U_R(2)$ symmetry. Further Feynman rules for QFT of Coulomb interaction of 2D graphite have been given and applied to the vacuum polarization and renormalization of effective Coulomb interaction constant and electron self energy which has important implication in the renormalization group analysis of g and v_f [6].

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